

SG No. 180 D_6^4 $P6_222$ [hexagonal]

* plus set: $+ [0, 0, 0]$

Table 1: Wyckoff site: 3a, site symmetry: 222

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 8, 11]$
2	$[0, 0, \frac{2}{3}]$	$[2, 5, 7, 10]$
3	$[0, 0, \frac{1}{3}]$	$[3, 6, 9, 12]$

Table 2: Wyckoff site: 3b, site symmetry: 222

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 4, 8, 11]$
2	$[0, 0, \frac{1}{6}]$	$[2, 5, 7, 10]$
3	$[0, 0, \frac{5}{6}]$	$[3, 6, 9, 12]$

Table 3: Wyckoff site: 3c, site symmetry: 222

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 8, 11]$
2	$[0, \frac{1}{2}, \frac{2}{3}]$	$[2, 5, 7, 10]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{3}]$	$[3, 6, 9, 12]$

Table 4: Wyckoff site: 3d, site symmetry: 222

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 8, 11]$
2	$[0, \frac{1}{2}, \frac{1}{6}]$	$[2, 5, 7, 10]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{5}{6}]$	$[3, 6, 9, 12]$

Table 5: Wyckoff site: 6e, site symmetry: 2..

No.	position	mapping
1	$[0, 0, z]$	$[1, 4]$
2	$[0, 0, z + \frac{2}{3}]$	$[2, 5]$
3	$[0, 0, z + \frac{1}{3}]$	$[3, 6]$
4	$[0, 0, \frac{2}{3} - z]$	$[7, 10]$
5	$[0, 0, -z]$	$[8, 11]$

continued ...

Table 5

No.	position	mapping
6	$[0, 0, \frac{1}{3} - z]$	[9, 12]

Table 6: Wyckoff site: 6f, site symmetry: $2..$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 4]
2	$[0, \frac{1}{2}, z + \frac{2}{3}]$	[2, 5]
3	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{3}]$	[3, 6]
4	$[0, \frac{1}{2}, \frac{2}{3} - z]$	[7, 10]
5	$[\frac{1}{2}, 0, -z]$	[8, 11]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{3} - z]$	[9, 12]

Table 7: Wyckoff site: 6g, site symmetry: $.2.$

No.	position	mapping
1	$[x, 0, 0]$	[1, 8]
2	$[0, x, \frac{2}{3}]$	[2, 7]
3	$[-x, -x, \frac{1}{3}]$	[3, 9]
4	$[-x, 0, 0]$	[4, 11]
5	$[0, -x, \frac{2}{3}]$	[5, 10]
6	$[x, x, \frac{1}{3}]$	[6, 12]

Table 8: Wyckoff site: 6h, site symmetry: $.2.$

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1, 8]
2	$[0, x, \frac{1}{6}]$	[2, 7]
3	$[-x, -x, \frac{5}{6}]$	[3, 9]
4	$[-x, 0, \frac{1}{2}]$	[4, 11]
5	$[0, -x, \frac{1}{6}]$	[5, 10]
6	$[x, x, \frac{5}{6}]$	[6, 12]

Table 9: Wyckoff site: 6i, site symmetry: $..2$

No.	position	mapping
1	$[x, 2x, 0]$	[1, 11]
2	$[-2x, -x, \frac{2}{3}]$	[2, 10]

continued ...

Table 9

No.	position	mapping
3	$[x, -x, \frac{1}{3}]$	[3,12]
4	$[-x, -2x, 0]$	[4,8]
5	$[2x, x, \frac{2}{3}]$	[5,7]
6	$[-x, x, \frac{1}{3}]$	[6,9]

Table 10: Wyckoff site: 6j, site symmetry: $\dots 2$

No.	position	mapping
1	$[x, 2x, \frac{1}{2}]$	[1,11]
2	$[-2x, -x, \frac{1}{6}]$	[2,10]
3	$[x, -x, \frac{5}{6}]$	[3,12]
4	$[-x, -2x, \frac{1}{2}]$	[4,8]
5	$[2x, x, \frac{1}{6}]$	[5,7]
6	$[-x, x, \frac{5}{6}]$	[6,9]

Table 11: Wyckoff site: 12k, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z + \frac{2}{3}]$	[2]
3	$[-x + y, -x, z + \frac{1}{3}]$	[3]
4	$[-x, -y, z]$	[4]
5	$[y, -x + y, z + \frac{2}{3}]$	[5]
6	$[x - y, x, z + \frac{1}{3}]$	[6]
7	$[y, x, \frac{2}{3} - z]$	[7]
8	$[x - y, -y, -z]$	[8]
9	$[-x, -x + y, \frac{1}{3} - z]$	[9]
10	$[-y, -x, \frac{2}{3} - z]$	[10]
11	$[-x + y, y, -z]$	[11]
12	$[x, x - y, \frac{1}{3} - z]$	[12]